

Effective Exchange Interactions for Bad Metals and Implications for Iron-based Superconductors

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The experimentally observed bad metal behavior in parent iron pnictides and chalcogenides suggests that these systems contain strong electronic correlations and are on the verge of a metal-to-insulator transition. The magnetic excitations in this bad-metal regime mainly derive from the incoherent part of the electronic spectrum away from the Fermi energy. We present a microscopic study of the exchange interactions in such a regime within a slave rotor approach. We find that the exchange interaction is maximized near the Mott transition. Generalizations to the multi-orbital case are discussed, as are the implications for the strength of superconducting pairing amplitude in the iron-based superconductors.

Introduction: Superconductivity in the iron pnictides and chalcogenides occurs at the border of antiferromagnetic order [1, 2]. For an understanding of the superconductivity, it is important to characterize the magnetism. An important clue for the latter is that the parent iron pnictides are bad metals. Their electrical resistivity at room temperature is very large, reaching the Mott-Ioffe-Regel limit ($k_F \ell < 2\pi$) [3, 4]. Optical conductivity measurements show a large suppression of the Drude weight [5], which suggests that the majority of the electronic excitations lives in the incoherent part away from the Fermi energy and the system is in proximity to a Mott insulator [6–8]. The role of the correlation effects is further highlighted by the observation of both the insulating states [9–13] and an orbital-selective Mott phase [14, 15] in a number of iron chalcogenides and it has also been emphasized from a variety of perspectives [16, 17, 19–29].

When the majority of the single-particle excitations are incoherent, they give rise to quasi-localized moments, which are coupled with each other through frustrating exchange interactions [6, 18–21]. This provides a natural basis to understand the large spin spectral weight observed in both the iron pnictides [30] and iron chalcogenides [31–34].

In this work, we study the exchange interactions in the bad-metal regime. While it is standard to derive superexchange interactions in the Mott localized regime, the microscopic basis for the exchange interactions in the regime of bad metals is much less understood. Here we show how such exchange interactions can be derived in a microscopic framework, using the slave-rotor approach [35, 36]. Important for our analysis is that this approach already contains incoherent excitation spectra at the saddle-point level. We show how such incoherent spectra can be integrated out to yield an exchange interaction, not only for the localized side but also in the bad-metal regime. As a consequence, we show that the exchange interaction is maximized near the Mott transition.

Slave-Rotor Approach: We consider the Hubbard model on a square lattice with only nearest-neighbor hopping

$$H_{HM}(d) = \sum_i H_{at}(i) - \sum_{ij,\alpha} (t_{ij} d_{i\alpha}^\dagger d_{j\alpha} + h.c.), \quad (1)$$

in which

$$H_{at}(i) = \frac{U}{2} \left(\sum_\alpha d_{i\alpha}^\dagger d_{i\alpha} - N/2 \right)^2,$$

α is the spin/orbital index running from $\alpha = 1, \dots, N$, with $N=2$ for the one-band model. For definiteness, we will consider a square lattice, and only hopping between nearest-neighbor (*n.n.*) sites, $\langle ij \rangle$. In the slave-rotor representation [36], $d_{i\alpha} \equiv f_{i\alpha} e^{-i\theta_i}$, with a constraint expressed in terms of the angular momentum $\hat{L}_i = -i\partial_{\theta_i}$:

$$\hat{L}_i = \sum_\alpha (f_{i\alpha}^\dagger f_{i\alpha} - 1/2). \quad (2)$$

In place of the phase field one could work with the complex field $e^{i\theta_i} = X_i$, with the additional constraint

$$|X_i|^2 = 1. \quad (3)$$

The two constraints are enforced by introducing two Lagrangian multipliers, h_i and λ_i . A saddle-point arises when one generalizes each X_i to M species so that its symmetry becomes $O(2M)$, scales the hopping t_{ij} to $1/M$, and take the large (N, M) limit with a fixed ratio M/N . In our analysis below, we will write our equations for $N = M = 2$.

Using $\partial_\tau \theta_i = -iX_i^* \partial_\tau X_i$, we have the Lagrangian

$$\begin{aligned} \mathcal{L}_{HM} = & \sum_{i,\alpha} f_{i\alpha}^\dagger (\partial_\tau + h_i) f_{i\alpha} + \sum_i \left(\frac{|\partial_\tau X_i|^2}{U} \right. \\ & + \frac{h_i}{U} (X_i^* \partial_\tau X_i - h.c.) + \lambda_i (|X_i|^2 - 1) \Big) \\ & + \sum_{ij,\alpha} (t_{ij} f_{i,\alpha}^\dagger f_{j,\alpha} X_i X_j^* + h.c.). \end{aligned} \quad (4)$$

Note that $\frac{U}{2} \sum_i \hat{L}_i^2 = \frac{|\partial_\tau X_i|^2}{2U}$; we have rescaled U to $U/2$ in (4) to preserve the correct atomic limit[35].

The saddle point [36, 37] corresponds to decoupling the spinon-boson coupling term via

$$\begin{aligned} Q_{f,ij} &= \langle X_j^* X_i \rangle, \\ Q_{X,ij} &= \langle \sum_\alpha f_{j\alpha}^\dagger f_{i\alpha} \rangle. \end{aligned} \quad (5)$$

The Lagrangian \mathcal{L}_{HM} is decoupled into two parts:

$$\mathcal{L}_{MF,f} = \sum_{i,\alpha} (f_{i\alpha}^\dagger (\partial_\tau + h_i) f_{i\alpha} + t \sum_{\langle ij \rangle, \alpha} (Q_f f_{i\alpha}^\dagger f_{j\alpha} + h.c.)), \quad (6)$$

$$\begin{aligned} \mathcal{L}_{MF,X} &= \sum_i \left(\frac{|\partial_\tau X_i|^2}{U} + \frac{h}{U} (X_i^* \partial_\tau X_i - h.c.) \right. \\ &\quad \left. + \lambda_i |X_i|^2 \right) + t \sum_{\langle ij \rangle} (Q_X X_i X_j^* + h.c.). \end{aligned} \quad (7)$$

The diagrams shown in Fig. (1a) correspond to the saddle point (see below). From here on, we drop the ij index for t and $Q_{f(X)}$ for notational simplicity. Then the spinon and X -field Green's functions at the saddle-point level read

$$G_f(\omega; \mathbf{k}) = (i\omega + h - Q_f \epsilon_{\mathbf{k}})^{-1}, \quad (8)$$

$$G_X(\nu; \mathbf{k}) = (\nu^2/U + 2ih\nu/U + \lambda + Q_X \epsilon_{\mathbf{k}})^{-1}, \quad (9)$$

where $\epsilon_{\mathbf{k}} = -2t(\cos(k_x) + \cos(k_y))$ is the bare lattice dispersion function. For the saddle point solution, the Lagrangian multipliers become uniform: $h_i \rightarrow h$ and $\lambda_i \rightarrow \lambda$. The self-consistent equation which determines λ reads

$$\int \frac{d^2 k}{(2\pi)^2} \sum_\nu G_X(\nu; \mathbf{k}) = 1. \quad (10)$$

The h is determined by $\langle \hat{L} \rangle = \sum_\alpha (\langle f_{i\alpha}^\dagger f_{i\alpha} \rangle - 1/2)$. For the half-filling case we consider, $h = 0$ for arbitrary U .

In both the insulating phase and the metallic phase, the spinons are always treated as free fermions at half-filling. We find $Q_X = \langle \sum_\alpha f_{i\alpha}^\dagger f_{j\alpha} \rangle = 8/\pi^2$, irrespective of U . Thus self-consistency is automatically satisfied. Q_f in general decays with increasing U , and in the large- U limit $Q_f \simeq 2/U$. The Mott transition is realized when U reaches U_c where $(\lambda + Q_X \epsilon_{\mathbf{k}=0})$ vanishes, so that the X -field starts to condense. For $U < U_c$, we can divide the rotor field into a condensate and an incoherent component: $X_i \rightarrow X_i^0 + X_i'$ and, correspondingly, the X -field Green's function may be written as

$$G_X(\nu; \mathbf{k}) = Z \delta(\nu) \delta(\mathbf{k}) + G_{X,\text{inc}}, \quad (11)$$

where $G_{X,\text{inc}} = \langle X_{\mathbf{k}}^* X_{\mathbf{k}}' \rangle = (\nu^2/U + \lambda_C + Q_X \epsilon_{\mathbf{k}})^{-1}$ and $Z = (X_i^0)^2$. In the metallic phase, $\lambda = \lambda_C$ remains a

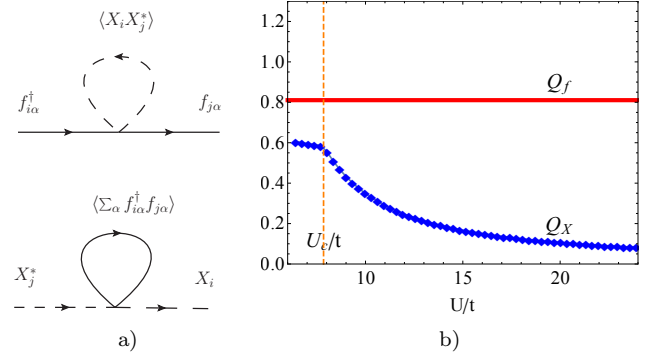


FIG. 1. (a) Feynman diagrams corresponding to the saddle point equations; (b) The self-consistent parameters Q_f and Q_X plotted as function of U/t .

constant, determined by $\lambda_C = -Q_X \epsilon_{\mathbf{k}=0}$. Then from Eq. (10), we find

$$Z = 1 - \sqrt{U/U_c}, \quad (12)$$

with U_c is determined from $\int \frac{d\nu d^2 k}{(2\pi)^3} (\nu^2/U_c + \lambda_C + Q_X \epsilon_{\mathbf{k}})^{-1} = 1$. The spinon's Green's function Eq. (8) remains the same (up to the renormalization factor Q_f). The division of the d -electron excitations into coherent and incoherent parts is thus realized by separating the rotor field X into a condensate and a fluctuating part. The parameters Q_f and Q_X computed numerically as function of U/t are shown in Fig. (1b).

Exchange Interaction from Integrating Out Incoherent Excitations: Beyond the saddle point, the spinon and rotor fields are coupled. To introduce these couplings, we consider Eq. (4) diagrammatically. \mathcal{L}_{HM} contains various bare interaction vortices as shown in Fig. (2a). The most important is the first, a spinon-rotor vortex; it corresponds to the hopping of the physical electrons. The others come from the constraints being enforced by the Lagrangian multiplier fields.

We first (formally) integrate out either the spinons ($f_{i\alpha}$ s) or the rotors (X_i s) from the full \mathcal{L}_{HM} of Eq. (4) to obtain effective actions $S^{\text{eff},X}(X_i)$ or $S^{\text{eff},f}(f_{i\alpha})$:

$$S^{\text{eff},f} = S^{0,f} - \ln \det \left[\begin{pmatrix} (G_X^0)^{-1} & t_{ij} \sum f_{i\alpha}^\dagger f_{j\alpha} \\ t_{ij} \sum f_{j\alpha}^\dagger f_{i\alpha} & (G_f^0)^{-1} \end{pmatrix} \right]_{i,j}, \quad (13)$$

$$S^{\text{eff},X} = S^{0,X} - \ln \det \left[\begin{pmatrix} (G_f^0)^{-1} & t_{ij} X_i^* X_j \\ t_{ij} X_j^* X_i & (G_X^0)^{-1} \end{pmatrix} \right]_{i,j}. \quad (14)$$

The $\ln \det[\dots]$ can be expanded in orders of t to generate effective hoppings and interactions. We take a renormalized expansion, so that G_f^0 and G_X^0 are replaced by G_f and G_X . To the lowest order in t , we only have the Feynman diagrams shown in Fig. (1a), which give rise

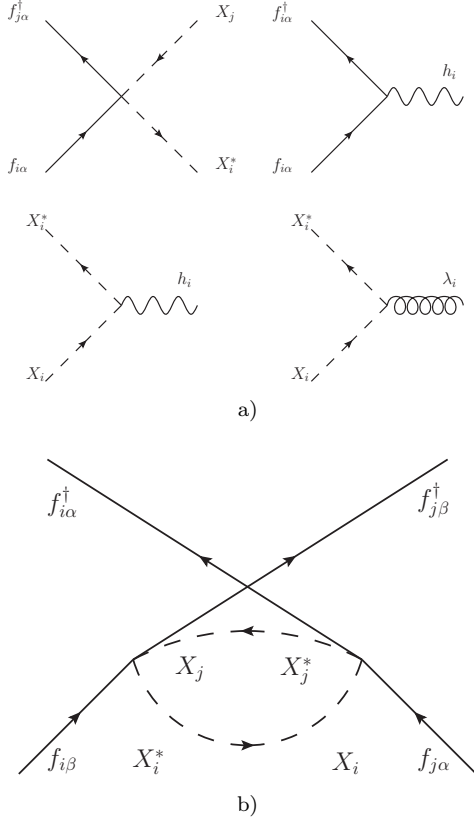


FIG. 2. (Color online) (a) Bare interaction vortices. (b) Feynman diagram for the effective spin exchange interaction.

to the saddle point where G_f and G_X are computed self-consistently. Again, for the metallic phase, we need to decompose the rotor fields into a condensate component and a fluctuating component: $X_i \rightarrow X_i' + X_i^0$.

For $S^{\text{eff},f}$ at $\mathcal{O}(t^2)$, we have the exchange vortex shown in Fig. (2b). This diagram yields a Heisenberg exchange interaction.

$$\begin{aligned} H_{f;\text{ex}} &= \frac{J_{\text{ex}}}{2} \sum_{\langle ij \rangle} \sum_{\alpha, \beta} f_{i\alpha}^\dagger f_{i\beta} f_{j\beta}^\dagger f_{j\alpha} \\ &= J_{\text{ex}} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \end{aligned} \quad (15)$$

where the factor 1/2 is because it is the second order term of the cumulant expansion. (We have ignored an additive constant in the last equality.) The exchange interaction is determined by the rotor bubble

$$J_{\text{ex}} = \int \frac{d\nu}{2\pi} G_X(\nu; i, i) G_X(\nu; j, j), \quad (16)$$

where $G_X(\nu; i, i) = \int \frac{d^2k}{(2\pi)^2} G_X(\nu; \mathbf{k})$. Note that, this exchange interaction operates in the spin sector, whose energies are low compared to the energies of the incoherent poles of the slave rotors (see below). This

makes the equal-time exchange interaction to be essentially the same as the static exchange interaction, for which Eq. (16) describes.

For latter reference, we contrast the above with a bare perturbative expansion. The latter is based on the following bare atomic actions and bare Green's functions of the spinons and rotors:

$$\begin{aligned} S^{0,f} &= \int d\tau \mathcal{L}^{0,f} = \int d\tau \sum_{i,\alpha} f_{i\alpha}^\dagger \partial\tau f_{i\alpha}, \\ S^{0,X} &= \int d\tau \mathcal{L}^{0,X} = \int d\tau \sum_i \left(\frac{|\partial\tau X_i|^2}{U} + \lambda |X_i|^2 \right), \\ G_X^0(\nu; i, j) &= \delta_{ij} (\nu^2/U + \lambda)^{-1}, \\ G_f^0(\omega; i, j) &= \delta_{ij} (i\omega)^{-1}. \end{aligned} \quad (17) \quad (18)$$

In this procedure, we can also determine an exchange interaction, $J_{\text{ex}}^{\text{bare}}$, from Eq. (16) with G_X replaced by G_X^0 .

Exchange Interaction on the Insulating Side: When U is significantly larger than U_c , the rotor spectrum has a large gap around $\omega = 0$, and two peaks around $\pm U\mathcal{O}(1)$ respectively. The latter characterizes incoherent electronic excitations, which are responsible for $J_{\text{ex}} \sim 1/U$ behavior. Numerical results for large- U s are shown in the inset of Fig. (4), where we also plot the ratio $J_{\text{ex}}/(\gamma t^2/U)$ as a function of U in which γ is determined by $J_{\text{ex}}/(\gamma t^2/U)|_{U \rightarrow \infty} = 1$ to compare with the standard super-exchange interaction. Here we do find $\gamma = 4$, in agreement with the standard result. Note that, the behavior at large U can be qualitatively seen by computing the rotor bubble function with the bare Green's function of the rotors: $J_{\text{ex}}^{\text{bare}}(U \rightarrow \infty) = \int \frac{d\nu}{2\pi} G_X^0(i\nu; i, i) G_X^0(i\nu; j, j)$. Using $\lambda_{U \rightarrow \infty} = U/4$ determined from Eq. (10), we find $J_{\text{ex}}^{\text{bare}} = \frac{\gamma t^2}{U}$. Though $\gamma = 2$ (as opposed to 4 above), $J_{\text{ex}}^{\text{bare}}$ does capture the t^2/U dependence.

Exchange Interaction in the Bad Metal Regime and across the Metal-Insulator Transition: When U approaches U_c from above, the evolution of the rotor spectral function (integrated over \mathbf{k}) is illustrated by the results shown in Fig. (3) for $U/U_c = 1.25, 1.1$. The incoherent peaks are still well-defined, but the peak locations naturally shift towards smaller ω . Therefore J_{ex} increases as $U \rightarrow U_c^+$.

Moving into the bad-metal regime, where $U < U_c$, the coherent electron weight Z is non-zero but still small. Importantly, the incoherent peaks remain in the rotor spectral function, as illustrated by the results shown in Fig. (3) for $U/U_c = 0.9, 0.75, 0.5$. We still have well-defined exchange interaction, J_{ex} from integrating out the incoherent spectra. Importantly,

$$\begin{aligned} J_{\text{ex}} &= \int \frac{d\nu}{2\pi} G_{X,\text{inc}}(\nu; i, i) G_{X,\text{inc}}(\nu; j, j) \\ &= \sqrt{\frac{U}{U_c}} \int \frac{d\nu'}{2\pi} G_{X,c}(\nu'; i, i) G_{X,c}(\nu'; j, j) \\ &= J_{\text{ex}}(U_c)(1 - Z), \end{aligned} \quad (19)$$

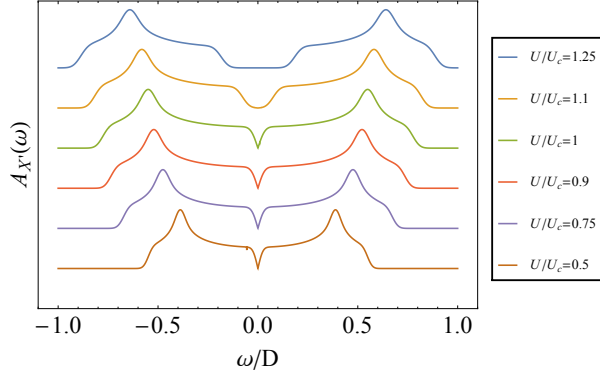


FIG. 3. (Color online) The incoherent spectral function of the slave rotor field plotted vs. ω/D for $U/U_c = 1.25, 1.1, 1, 0.9, 0.75, 0.5$ respectively. Here, D is the electron bandwidth $D = 8t$, and each curve is shifted by a different constant. When U is larger than U_c , the rotor spectral weight has a gap around $\omega = 0$. In addition, it has two peaks near $\pm U\mathcal{O}(1)$, which correspond to two incoherent poles of the rotor Green's function. These poles persist into the bad metal regime across the Mott transition, as can be seen from the results for $U/U_c < 1$.

where $G_{X,c}(\nu'; \mathbf{k}) = (\nu'^2/U_c + \lambda_c + Q_X \epsilon_{\mathbf{k}})^{-1}$ is transformed from $G_{X,\text{inc}}(\nu; \mathbf{k})$ by letting $\nu' = \nu\sqrt{U_c/U}$. Because the spectral weight in the incoherent part is lost to the coherent part, the exchange interaction will decrease as U decreases from U_c .

We therefore expect that J_{ex} will be maximized around U_c . This is indeed seen in the calculated result near the Mott transition, shown in Fig. (4).

Discussions: The slave-rotor method can also be generalized to the multi-orbital cases [36, 38]. From integrating out the incoherent spectra of the slave rotors, we will again get four-spinon interactions. These interactions are more complex, because the appropriate spinon bilinears may not only involve the spin degrees of freedom, but also the orbital ones. The form of the latter will depend on the filling factors. Here we will concentrate on the interactions that involve only the spins, in which case the effective interaction will be the on-site Hund's couplings and intersite exchange interactions of the following form [6]: $\sum_{ij,\tau\tau'} J_{ij}^{\tau\tau'} \mathbf{S}_i^\tau \cdot \mathbf{S}_j^{\tau'}$, where τ, τ' label the orbitals. The exchange interaction forms a matrix in the orbital basis. The individual matrix element, $J_{ij}^{\tau\tau'}$, can be calculated within the framework we have presented here, and will depend on U in a way similar to our results presented above for the single-orbital case.

We have used the slave rotor approach here as a means to capture the incoherent part of the electron spectral weight. An attractive alternative approach is a slave-spin method, either in the Z_2 form [40] or in the $U(1)$ form [41]. The $U(1)$ formulation, in particular, properly describes the Mott insulating phase and should therefore be able to capture the incoherent part of the elec-

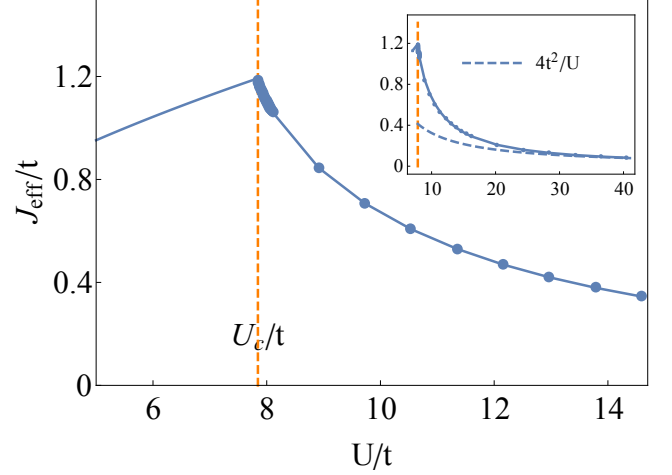


FIG. 4. (Color online) The calculated J_{ex} plotted as a function of U/t from the bad-metal regime to the insulating side. The exchange interaction is seen to be maximized around the Mott transition. The inset shows J_{ex} on the insulating side up to large values of U/t ; the axes are the same as in the main plot. The dashed line corresponds to the standard result for the large- U limit, $J_{\text{ex}} \simeq \gamma t^2/U$ with $\gamma = 4$.

tron spectral weight in a similar fashion. This approach could be advantageous to understanding the dependence of the exchange interactions on the Hund's coupling [21]. Nonetheless, our procedure presented here already provides the conceptual basis for deriving the exchange interactions in the bad-metal regime (in other words, not just on the insulating side).

Finally, we have focused on the Heisenberg exchange interaction. Our procedure also contains processes for multi-spin exchange interactions. These include both the bi-quadratic couplings and ring-exchange interactions.

Implications for the Iron-based Superconductors: Superconductivity can be driven by the short-range exchange interactions. Recent work by some of the co-authors here [39] have shown that the pairing amplitude increases with increasing J_{ex}/D^* , where D^* is the renormalized bandwidth. Since D^* decreases as the Mott transition is approached, and J_{ex} is maximized there, the superconducting pairing amplitude is expected to be the largest near the boundary of localization and delocalization.

To summarize, we have presented a microscopic approach to determine the exchange interactions in the bad metal regime. From concrete calculations, we have demonstrated that the exchange interaction is the largest near the boundary of localization and delocalization. Correspondingly, superconductivity driven by short-range interactions is expected to have the largest pairing amplitude in such a regime.

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- [1] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, *J. Am. Chem. Soc.* **130**, 3296 (2008).
- [2] C. de la Cruz, Q. Huang, J. W. Lynn, J. Li, W. Ratcliff, J. L. Zarestky, H. a. Mook, G. F. Chen, J. L. Luo, N. L. Wang, and P. Dai, *Nature* **453**, 899 (2008).
- [3] E. Abrahams and Q. Si, *J. Phys. Condens. Matter* **23**, 223201 (2011).
- [4] N. E. Hussey, K. Takenaka, and H. Takagi, *Philoso. Mag.* **84**, 2847 (2004).
- [5] M. M. Qazilbash, J. J. Hamlin, R. E. Baumbach, L. Zhang, D. J. Singh, M. B. Maple, and D. N. Basov, *Nat. Phys.* **5**, 647 (2009).
- [6] Q. Si and E. Abrahams, *Phys. Rev. Lett.* **101**, 076401 (2008).
- [7] Q. Si, E. Abrahams, J. Dai, and J.-X. Zhu, *New J. Phys.* **11**, 045001 (2009).
- [8] K. Haule, J. H. Shim, and G. Kotliar, *Phys. Rev. Lett.* **100**, 226402 (2008).
- [9] M.-H. Fang, H.-D. Wang, C.-H. Dong, Z.-J. Li, C.-M. Feng, J. Chen, and H. Q. Yuan, *Europhys. Lett.* **94**, 27009 (2011).
- [10] P. Gao, R. Yu, L. Sun, H. Wang, Z. Wang, Q. Wu, M. Fang, G. Chen, J. Guo, C. Zhang, D. Gu, H. Tian, J. Li, J. Liu, Y. Li, X. Li, S. Jiang, K. Yang, A. Li, Q. Si, and Z. Zhao, *Phys. Rev. B* **89**, 094514 (2014).
- [11] R. Yu, J.-X. Zhu, and Q. Si, *Phys. Rev. Lett.* **106**, 186401 (2011).
- [12] E. Dagotto, *Rev. Mod. Phys.* **85**, 849 (2013).
- [13] J.-X. Zhu, R. Yu, H. Wang, L. L. Zhao, M. D. Jones, J. Dai, E. Abrahams, E. Morosan, M. Fang, and Q. Si, *Phys. Rev. Lett.* **104**, 216405 (2010).
- [14] M. Yi, D. Lu, R. Yu, S. Riggs, J.-H. Chu, B. Lv, Z. Liu, M. Lu, Y.-T. Cui, M. Hashimoto, S.-K. Mo, Z. Hussain, C. Chu, I. Fisher, Q. Si, and Z.-X. Shen, *Phys. Rev. Lett.* **110**, 067003 (2013).
- [15] R. Yu and Q. Si, *Phys. Rev. Lett.* **110**, 146402 (2013).
- [16] C. Fang, H. Yao, W.-F. Tsai, J. Hu, and S. a. Kivelson, *Phys. Rev. B* **77**, 224509 (2008).
- [17] C. Xu, M. Müller, and S. Sachdev, *Phys. Rev. B* **78**, 020501 (2008).
- [18] T. Yildirim, *Phys. Rev. Lett.* **101**, 057010 (2008).
- [19] F. Ma, Z.-Y. Lu, and T. Xiang, *Phys. Rev. B* **78**, 224517 (2008).
- [20] M. Han, Q. Yin, W. Pickett, and S. Savrasov, *Phys. Rev. Lett.* **102**, 107003 (2009).
- [21] M. J. Calderon, G. Leon, B. Valenzuela, and E. Bascones, *Phys. Rev. B* **86**, 104514 (2012).
- [22] K. Seo, B. A. Bernevig, and J. Hu, *Phys. Rev. Lett.* **101**, 206404 (2008).
- [23] W.-Q. Chen, K.-Y. Yang, Y. Zhou, and F.-C. Zhang, *Phys. Rev. Lett.* **102**, 047006 (2009).
- [24] A. Moreo, M. Daghofer, J. Riera, and E. Dagotto, *Phys. Rev. B* **79**, 134502 (2009).
- [25] W. Lv, F. Krüger, and P. Phillips, *Phys. Rev. B* **82**, 045125 (2010).
- [26] G. Uhrig, M. Holt, J. Oitmaa, O. Sushkov, and R. Singh, *Phys. Rev. B* **79**, 092416 (2009).
- [27] H. Ishida and A. Liebsch, *Phys. Rev. B* **81**, 054513 (2010).
- [28] G. Giovannetti, C. Ortix, M. Marsman, M. Capone, J. van den Brink, and J. Lorenzana, *Nat. Commun.* **2**, 398 (2011).
- [29] E. Bascones, B. Valenzuela, and M. J. Calderón, *Phys. Rev. B* **86**, 174508 (2012).
- [30] M. Wang, C. Fang, D.-X. Yao, G. Tan, L. W. Harriger, Y. Song, T. Netherton, C. Zhang, M. Wang, M. B. Stone, W. Tian, J. Hu, and P. Dai, *Nat. Commun.* **2**, 580 (2011).
- [31] W. Bao, Q.-Z. Huang, G.-F. Chen, D.-M. Wang, J.-B. He, and Y.-M. Qiu, *Chin. Phys. Lett.* **28**, 086104 (2011).
- [32] J. Zhao, H. Cao, E. Bourret-Courchesne, D.-H. Lee, and R. J. Birgeneau, *Phys. Rev. Lett.* **109**, 267003 (2012).
- [33] D. G. Free and J. S. O. Evans, *Phys. Rev. B* **81**, 214433 (2010).
- [34] E. E. McCabe, C. Stock, E. E. Rodriguez, a. S. Wills, J. W. Taylor, and J. S. O. Evans, *Phys. Rev. B* **89**, 100402 (2014).
- [35] S. Florens and A. Georges, *Phys. Rev. B* **66**, 165111 (2002).
- [36] S. Florens and A. Georges, *Phys. Rev. B* **70**, 035114 (2004).
- [37] S.-S. Lee and P. A. Lee, *Phys. Rev. Lett.* **95**, 036403 (2005).
- [38] W.-H. Ko and P. A. Lee, *Phys. Rev. B* **83**, 134515 (2011).
- [39] R. Yu, P. Goswami, Q. Si, P. Nikolic, and J.-X. Zhu, *Nat. Commun.* **4**, 2783 (2013).
- [40] L. de’ Medici, A. Georges, and S. Biermann, *Phys. Rev. B* **72**, 205124 (2005).
- [41] R. Yu and Q. Si, *Phys. Rev. B* **86**, 085104 (2012).